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Dynamic and Static Modeling at Interfaces and Nanostructures

This seminar will be focused on some of the research performed during my PhD at the University of Bordeaux (France) and my postdoc at the Donostia International Physics Center in San Sebastian (Spain).

The rationalization of heterogeneous elementary processes is of great importance for several domains of research such as heterogeneous catalysis, hydrogen storage or plasma physics. In particular, systems involving recombination of hydrogen on tungsten surfaces are of current technological interest in the context of the ITER experimental fusion reactor as this metal is the main candidate for the divertors of the tokamaks. After presenting the conclusions of preliminary investigations of direct hydrogen recombination, the so-called Eley-Rideal (ER) process, on tungsten surfaces (W(100) and W(110))[1,2], the development of a many-adsorbate potential energy surface (PES) to account for surface coverage in abstraction dynamics will be discussed.[3]

Engineering of atomic and molecular nanostructures at surfaces has been widely attractive for a broad range of applications such as molecular electronics, memory and spintronic devices… Thus, the investigation of systems involving adsorption of organic molecules on metallic surfaces was my primary research activity during my postdoc in San Sebastian. Comparison of STM data (group of Prof. Klaus Kern at Max Planck Institute Stuttgart) with DFT calculations results have allowed to unravel STM driven single molecule reaction mechanisms of two different analogs of pentacene: i) the bipolar conductance switching mechanism of anthradithiophene[4] and ii) the electric-field-driven direct desulfurization of tetracenothiophene.[5]

[1] Pétuya, R. *et al.* **2014** *Journal of Chemical Physics*, 141(110), 024701 1-10.
[2] Pétuya, R. *et al.* **2014** *The Journal of Physical Chemistry C*, 118(100), 11704.
[3] Pétuya, R. *et al.* **2015** *The Journal of Physical Chemistry C*, 119(6), 3171-3179.
[4] Borca, B., *et al.* **2015** *ACS Nano*, 9(12), 12506-12512.
[5] Borca, B., et al. **2017** *ACS Nano*, 11(5), 4703-4709.